

June 2017

# Science & Technology

REVIEW

TECHNOLOGY TRANSFER

## HALL OF FAME



*Also in this issue:*

**Entrepreneurship Takes Root**

**National Security Code Retooled for Industry**

**A New Way to Make High-Performance Composites**



## About the Cover

Since its founding, Lawrence Livermore has embraced its role as a venue for scientific research and development, a proving ground for new technology, and an advocate for transferring technology to the private sector. Livermore deliberately cultivates a culture of entrepreneurship to ensure that appropriate innovations enhance U.S. economic security. As the article beginning on p. 4 describes, the Laboratory has established an Entrepreneurs' Hall of Fame to recognize the most successful of these technologies and the researcher-entrepreneurs who created them. From pioneering laser peening and satellite imaging technology to computer simulations and cybersecurity, Hall of Fame inductees have made a lasting impact on U.S. industry. The Industrial Partnerships Office (IPO) has played a key role in these successes and today continues to assist Livermore scientists and engineers with the myriad aspects of technology transfer.



Cover design: Max Rodriguez and Alexandria Holmberg

## About S&TR

At Lawrence Livermore National Laboratory, we focus on science and technology research to ensure our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published eight times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

The Laboratory is operated by Lawrence Livermore National Security, LLC (LLNS), for the Department of Energy's National Nuclear Security Administration. LLNS is a partnership involving Bechtel National, University of California, Babcock & Wilcox, Washington Division of URS Corporation, and Battelle in affiliation with Texas A&M University. More information about LLNS is available online at [www.llnslc.com](http://www.llnslc.com).

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Prepared by LLNL under contract  
DE-AC52-07NA27344

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*S&TR*, a Director's Office publication, is produced by the Technical Information Department under the direction of the Office of Planning and Special Studies.

*S&TR* is available on the Web at [str.llnl.gov](http://str.llnl.gov)

Printed in the United States of America

Available from  
National Technical Information Service  
U.S. Department of Commerce  
5285 Port Royal Road  
Springfield, Virginia 22161

UCRL-TR-52000-17-6  
Distribution Category UC-99  
June 2017

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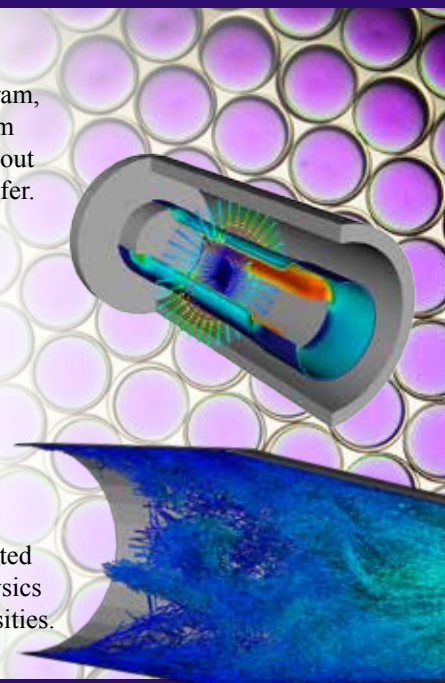
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### Theory for Crater Formation on Martian Moon

Physicists at Lawrence Livermore have demonstrated for the first time how an asteroid or comet impact could have created Stickney Crater on the Martian moon Phobos without obliterating the moon in the process. The dominant surface feature on Mars's largest moon, Stickney Crater spans 9 kilometers, stretching nearly halfway across Phobos (see photograph below). However, understanding the massive crater's formation has proven elusive until now.

"We have demonstrated, in a three-dimensional simulation, that the crater can be created without destroying the moon if the proper



porosity and resolution are used," says Megan Bruck Syal, a member of the Laboratory's planetary defense team and lead author of research published in

the October 24, 2016, edition of *Geophysical Research Letters*. The study showed that a range of possible solutions exists for the size and speed of the impactor, but Syal says one possible scenario is an object 250 meters across traveling close to 6 kilometers per second.

The research served as a benchmarking exercise for the team, which uses a Livermore-developed open-source code called Spheral to simulate various methods of deflecting potentially hazardous Earthbound asteroids. Bruck Syal points out, "Something as big and fast as what caused Stickney Crater would have a devastating effect on Earth. If NASA sees a potentially hazardous asteroid coming our way, it will be essential to make sure we are able to deflect it. We will only have one shot at it, and the consequences could not be higher. We do this type of benchmarking research to make sure our codes are right when they will be needed most."

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### Measuring Radiation Dose from Cancer Treatment

Lawrence Livermore scientists have developed a new technique using gene-expression analysis to measure internal radiation dose in cancer patients receiving targeted radiation therapy. Although dosimeters can be used to measure radiation dose externally, more precise dosimeters to assess internal dose do not exist.

In a paper published in the August 24, 2016, edition of *Radiation Research*, the Lawrence Livermore team—with collaborators at Purdue University, the University of California (UC) at San Francisco, UC Davis, and Houston Methodist Research

Institute—describes a technique to characterize internal exposure by using gene-expression assays to monitor changes at the molecular level. This sort of biological approach to measuring physical dosimetry is known as biodosimetry. The method was used to compare calculated internal dose with the modulation of selected RNA transcripts.

"This is a novel study, using whole blood collected from patients treated with a radiopharmaceutical, to characterize biomarkers that may be useful for better cancer treatment and biodosimetry," says coauthor Matt Coleman, a Livermore biologist and adjunct professor at UC Davis. "Our data indicate that RNA transcripts, which have been previously identified as biomarkers of external exposures in whole blood and radiotherapy patients, also are good early indicators of internal exposure." The technique also may be a valuable tool for first responders to triage individuals after a nuclear accident or for astronauts to monitor space radiation exposure while traveling to Mars.

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### Metamaterials Shrink When Heated

Livermore engineers, working with researchers from the University of Southern California, the Massachusetts Institute of Technology, Singapore University of Technology and Design, and the University of California at Los Angeles, have created three-dimensionally printed, lightweight materials exhibiting negative thermal expansion, that is, a tendency to shrink when heated. The materials are metamaterials—composites whose properties heavily rely upon their internal structure—and are described in a paper published in the October 21, 2016, edition of *Physical Review Letters*.

Researchers note the study may be the first experimental demonstration showing large tunability of negative thermal expansion in three Cartesian directions of microlattice structures. Printed from a polymer or polymer-copper composite that can flex inward, the microlattice structure contracts when exposed to heat over a range of tens to hundreds of degrees. Principal investigator Chris Spadaccini says, "Our metamaterials have thermomechanical properties not achievable in conventional bulk materials."

The metamaterials consist of beams surrounded by void space. When heated, some beams expand more than the others, causing the connecting points between each unit cell to pull inward and making the overall microlattice contract. Thermal expansion also can be zero or positive, depending on how the geometry and topology of the structure are engineered. Possible applications for such metamaterials include securing parts that tend to move out of alignment under varying heat loads, such as microchips and high-precision optical mounts.

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# A Tradition of Technological Breakthroughs with Commercial Success

Location, location, location. Real estate professionals might say Lawrence Livermore, perched on the eastern edge of California's Silicon Valley, is perfectly situated to participate in the nation's booming technology sector. Indeed, our national and global security missions require continual advancements in science and technology, and our researchers are regularly recognized for innovative achievements—particularly those with both security and industrial applications.

The Federal Laboratory Consortium for Technology Transfer (FLC) honors outstanding research and development (R&D) efforts across its network of more than 300 laboratories. Over the years, Livermore has earned several national FLC awards for Outstanding Technology Development, Outstanding Commercialization Success, Outstanding Partnerships, and Interagency Partnership. In the past decade, we have also won 28 FLC regional awards, most recently for WiBSAFE (wireless battery sensing and failure eliminator) and for our partnership with two companies licensing a geothermal silica-extraction technology. Livermore scientists also frequently receive annual R&D 100 awards for inventive technology, and 2016 was no exception. (See *S&TR*, January/February 2017, pp. 12–18.) The Laboratory placed 25th in Reuters' 2017 list of the world's most innovative research institutions, where rankings are determined by criteria such as scholarly and industry publications, academic citations, and the ratio of patents filed to patents granted.

Yet these accolades tell only part of the story. In fact, Livermore has a many-decades-long history of facilitating technology transfer and encouraging entrepreneurship. As the article beginning on p. 4 details, the Industrial Partnerships Office (IPO) recognizes some of our legacies in the Laboratory's Entrepreneurs' Hall of Fame, which boasts an impressive catalog of invention, collaboration, and determination. These 19 Hall of Fame alumni—5 of whom are profiled in the article—have made significant contributions to both the Laboratory and commercial markets. Their work evolves as industries change, and in many cases, their achievements continue to accumulate. Looking ahead to the next round of inductees, I am reminded that these success stories are evidence of our continuing journey of "Science on a Mission" in service to our nation.

IPO actively engages with industries to market Laboratory ideas. For instance, IPO helps researchers find commercial

opportunities and navigate their entrepreneurial journeys. IPO staff also manage a large portfolio of licenses and other agreements, which yield royalty income for the Laboratory, sustained success for inventors, and real-world solutions for urgent problems. This relationship is truly a win-win-win situation.

The Laboratory also invests in programs that educate prospective entrepreneurs about promoting, protecting, and evolving their ideas. One such program is Energy I-Corps, part of the Department of Energy's new National Laboratory Accelerator Program. (See the article beginning on p. 12.) Energy I-Corps provides a comprehensive approach to improving participants' business acumen. Program graduates find themselves better equipped to handle the rigors of writing an engaging business plan and selling their discovery to investors.

This issue also highlights current research beginning to make its way outside Laboratory gates. For instance, innovations in carbon fiber composites are leading to enhanced structures and other advancements to meet industry demands for stronger, more adaptable feedstocks in additive manufacturing. (See the article beginning on p. 16.) Another homegrown technology gaining traction with a wider audience is the three-dimensional multiphysics code ALE3D. (See the article beginning on p. 20.) ALE3D exemplifies the increased attention that Livermore simulation capabilities are receiving as more and more industries rely on high-performance computing to solve problems. Similar Laboratory-developed examples abound beyond the pages of this issue.

Livermore's technology-transfer reputation is built by leaders who understand industry needs and nurture emerging technologies, and by our researchers' constant pursuit of innovative solutions. As the Laboratory marks its 65th anniversary, we are renewing our commitment to strong industry relationships that will enable us to further contribute to the U.S. economy and bolster the nation's security. Our tradition of innovation—backed by the hard work, dedication, and intellect of our researchers—is indeed forging a brighter future for the nation.

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■ Thomas F. Gioconda is deputy director of Lawrence Livermore National Laboratory.



# Ready, Set, Innovate!

## ENTREPRENEURSHIP FLOURISHES AT THE LABORATORY



*Lawrence Livermore's Industrial Partnerships Office uses its technology-transfer expertise to help the Laboratory's successful innovators contribute to the nation's economy. These top inventors are enshrined in the Entrepreneurs' Hall of Fame.*

**G**REAT ideas percolate, evolving into even better ones. The best ideas can ultimately rise to the top and make a tangible difference in the nation—when given the right outlet. For close to 65 years, Lawrence Livermore has embraced all of these stages of innovation as a venue for scientific research and development, a proving ground for new technologies, and an advocate for transferring technology to the private sector. Livermore's culture of entrepreneurship ensures that innovations with broad applications find a purpose beyond Laboratory gates, providing economic benefit at the local, state, and national level.

Technology transfer, or the commercialization of an invention, is a complicated process. Wading through licensing agreements, nondisclosure contracts, and patent applications is only the beginning. Protecting intellectual property is critical, as are drafting a business plan, applying for funding, and formulating a go-to-market strategy. These tasks can seem daunting to a scientist or engineer whose day job is steeped in laboratory equipment or computer codes. Those who embark on the entrepreneurial journey often need help, which is where the Laboratory's Industrial Partnerships Office (IPO) comes in.

Livermore's concerted technology-transfer efforts began in the mid-1980s as part of its national security mission. IPO promotes Laboratory-developed technologies for commercial partners who identify opportunities and seek licenses or cooperative research and development agreements (CRADAs) to further shape the technology for market applications. (See *S&TR*, July/August 2008, pp. 4–11.) IPO Director Rich Rankin says, "The most challenging aspect of technology transfer is picking winners." Rankin's staff includes scientists and specialists in commercialization, intellectual property, product development, market analysis,

business, and law. Rankin continues, "Our expertise helps us figure out how best to invest limited time and resources in promising technology that positively impacts the nation's economy."

IPO has organized networking events with potential investors and cohosted educational seminars with universities and other laboratories. Staff also participate in conferences, student mentoring, and business development webinars. Other outreach activities include membership in national laboratory consortia, onsite collaboration at the Livermore Valley Open Campus, and engagement with the Department of Energy's Energy I-Corps and other parts of the National Laboratory Accelerator Program. (See *S&TR*, March 2015, pp. 4–10; and the article beginning on p. 12 in this issue.)

### **Secrets of Success**

IPO takes an end-to-end approach to entrepreneurship with initiatives that advise employees on everything from identifying a market need to finding a corporate partner who can transform the technology into a marketable product. For instance, the Entrepreneurs-in-Readiness Program connects Livermore entrepreneurs with seasoned experts from California's Silicon Valley. In addition to this program, the Laboratory uses the National Laboratory Entrepreneurship Academy at the University of California (UC) at Davis to educate scientists about the commercialization process. Serial entrepreneurs bring wisdom and fresh perspectives to early-stage technologies, often finding hidden potential or new ways of thinking about a technology's applications. These mentors can also help scientists tap into a network of investors and partners. IPO Deputy Director Roger Werne emphasizes the importance of a network for the aspiring entrepreneur. He says, "You must have advisors who can

provide insight into the market you're targeting." When the time is right, an employee may decide to create a startup or join an existing company to launch his or her product. IPO works with employees who wish to steer their careers in this direction. "Scientists and engineers can be naïve about what it takes to become commercially successful," says Werne. "Entering the marketplace is a gamble. Fortunately, Livermore's credibility in many industries means venture capitalists or angel investors will usually listen to what we have to say."

Although entrepreneurs may define success differently, success for IPO is measured by a license or CRADA to refine the technology for a commercial purpose. Eventually, a technology's impact in the market is measured by royalties on product sales. Annually, Livermore-developed technologies generate more than \$300 million in sales, earning the Laboratory more than \$8 million in licensing fees and royalties. With more than 1,000 active agreements and just as many patents and patent applications, IPO oversees upwards of 140 active commercial

licenses and CRADAs. These quantities also boast quality—to date, Livermore scientists have received 155 R&D 100 awards. Winning one of these prestigious awards is considered a respected achievement that also enhances marketability.

### A Cooperstown for Innovation

To recognize scientists whose inventiveness and entrepreneurial spirit have made significant impacts on both the Laboratory and the private sector, Werne worked with Laboratory Director Emeritus Bruce Tarter to establish the

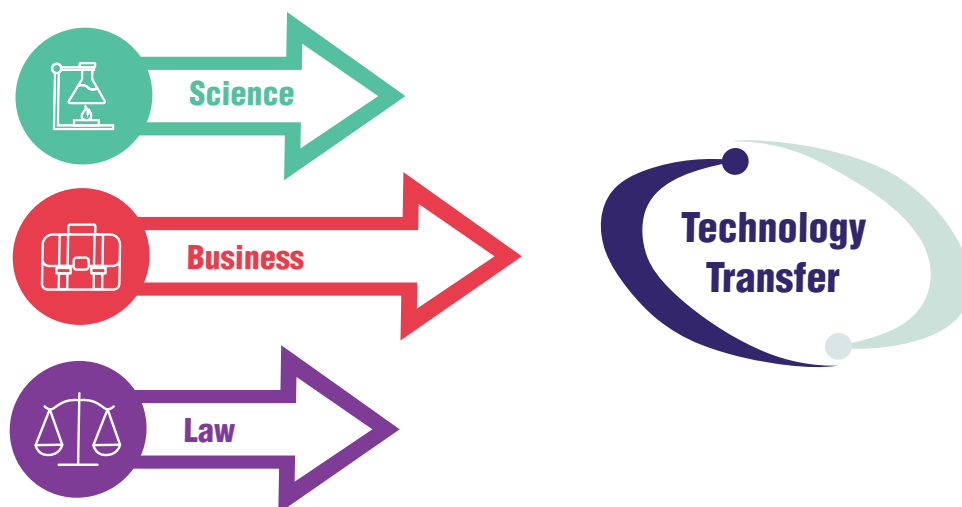


The Entrepreneurs' Hall of Fame, in Lawrence Livermore's Industrial Partnerships Office (IPO), recognizes successful entrepreneurs and their achievements.



Entrepreneurs' Hall of Fame (EHF) in 2012, coinciding with Livermore's 60th anniversary. Fifteen scientists were inducted in the inaugural class, with four more honored in 2015. (See *S&TR*, December 2012, p. 2; and *S&TR*, March 2015, p. 24.) Alone among national laboratories, Livermore's EHF benefits

IPO Director Rich Rankin defines technology transfer as the intersection of science, business, and law. He notes, "Our staff have experience in all of these areas."



## Making Waves in Varied Ways

Lawrence Livermore's Entrepreneurs' Hall of Fame (EHF) honors scientists whose efforts at the Laboratory led to successful technology transfers. Many EHF inductees have continued their work regionally in California's Silicon Valley, a hotbed of startups full of like-minded innovators looking for leading-edge solutions to a range of problems. For example, Michael Farmwald addressed crucial performance problems in supercomputing and electronic microprocessors at the Laboratory before transitioning to serial startups. After beginning his career at the Laboratory, Bruce McWilliams brought his physics expertise to the semiconductor industry, founding or joining multiple companies while evolving his unique multichip packaging technology and other semiconductor components. Similarly, David Tuckerman joined McWilliams at two startups before founding a consulting firm that connects venture capitalists and industrial clients. Tuckerman's background in engineering, computer science, and angel investments have enabled him to nurture a new generation of entrepreneurs.

Other EHF members have invented new products or improved existing tools. James Bryan, known as the "Father of Precision Engineering," developed a telescoping magnetic ball bar that provides high-precision machine tool calibration. Thomas McEwan's work with Livermore's Nova laser—a predecessor to the National Ignition Facility—led to the invention of an ultrasensitive radar system called micropower impulse radar. This radar can be found in a variety of applications for military personnel—including landmine detection systems and wall-penetrating radar—and for homeowners, such as stud finders and motion detectors. The technology has garnered multiple awards and continues to be one of Livermore's biggest royalty generators. In a surprising benefit for consumer products, Robert Parker's stockpile stewardship work in temperature sensors led to a breakthrough in liquid crystal technology, whose applications included the popular "Mood Rings" of the 1970s. Parker's later inventions include a self-contained solder joint system and a visual temperature-distribution indicator for cookware.

EHF brainpower has also boosted computer technology. Curtis Widdoes and Thomas McWilliams designed the first supercomputer in

the historic S-1 series, the Mark-1, and created the structured computer-aided logic design (SCALD) language to improve design processes. Computer engineer Jeffrey Rubin joined their effort to enhance and debug the system, and the three founded Valid Logic Systems to commercialize SCALD technology. All went on to pursue further innovations in hardware and software, and the industry took notice—McWilliams and Rubin's startup PathScale sold to Intel, while Widdoes's company, Logic Modeling Systems, was acquired by Synopsys.

Medical breakthroughs are also represented in the EHF. Fluorescence in situ hybridization (FISH), a method of binding molecules to nucleic acid fragments for easier detection of genetic sequences, was originally designed to evaluate radiation doses received by Hiroshima and Nagasaki survivors. With the Laboratory's help, Daniel Pinkel and Joe Gray licensed the technology to a commercial company. FISH is now a leading diagnostic technique for assessing radiation doses and other environmental exposures and has applications in genetic counseling and species identification.

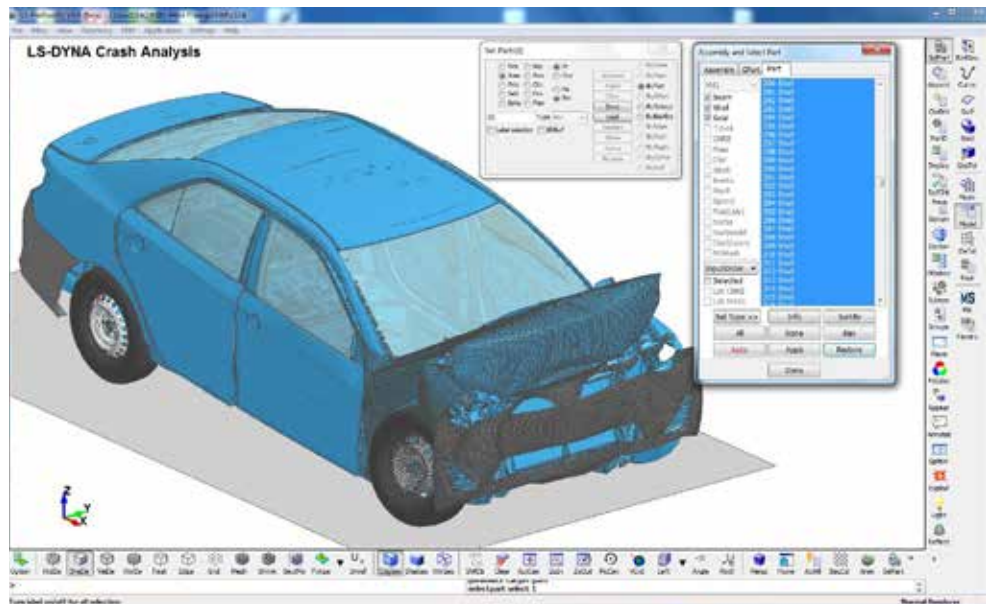
Advancements in another type of DNA analysis known as polymerase chain reaction (PCR) have come from multiple EHF inductees. Bill Colston and Fred Milanovich secured several patents, R&D 100 awards, and Laboratory Directed Research and Development Program funding for work that eventually led to a product called Droplet Digital PCR. The product divides a genetic specimen into thousands of equivalent samples for expanded testing and increased accuracy. Since commercialization, Droplet Digital PCR has penetrated the forensic science, DNA cloning, prenatal testing, and genetic analysis markets. (See *S&TR*, April/May 2017, pp. 4–12.)

Biomedical progress continues thanks to Allen Northrup, who used his expertise in microinstrumentation to create a silicon chip capable of rapidly copying billions of DNA samples via PCR. After successful deployment of biodetection field units in the wake of the 2001 anthrax attacks, the technology is now a mainstay of biotechnology, forensic analysis, and countering bioterrorism. Northrup's company, Cepheid, recently sold for \$4 billion.

the Laboratory as much as the scientists it honors. Werne notes, “The Hall of Fame is demonstrable evidence of the value of our work.”

EHF inclusion has three criteria—innovative technology, business acumen, and company value. Evaluating a prospective inductee takes time. Werne notes that companies typically need 10 to 20 years to achieve substantial success. By the time the Hall of Famers were officially honored, he says, “their mark in the commercial world had been made, and they had provided something of commercial value to the country.” The motto of the National Baseball Hall of Fame—“Preserving History, Honoring Excellence, Connecting Generations”—could also apply to these notable entrepreneurs. All spent several years at the Laboratory developing their technologies before exploring commercial opportunities. Many give back to the Laboratory by volunteering their time as mentors and advisors in IPO’s programs. According to Rankin, achievements honored by the EHF share a fundamental result: “These technologies impact more than the economy. They’ve changed how we live.” (See box on p. 7.)

John O. Hallquist invented finite-element code DYNA3D, released commercially as LS-DYNA. In 1987, he founded Livermore Software Technology Corporation, which holds 65 U.S. utility patents. (Photograph by Julie Russell.)



Although individuals carve their own paths, five EHF inductees in particular underscore several essential phases common to all entrepreneurial journeys.

### Phase 1: Develop the Product

In the early days of supercomputing, no existing code could predict the structural response of weapons impacting the ground prior to detonation. In the mid-1970s, John O. Hallquist was asked to develop simulation software with three-dimensional capabilities. Hallquist named his resultant 5,000-line code DYNA3D and later developed a two-dimensional version (DYNA2D) and other finite-element and visualization codes to simulate the mechanical behavior—bending, folding, collapse—of collision events. Hallquist

LS-DYNA models mechanical failure. The code has been used in the automotive industry to save billions of dollars and has greatly improved safety. A car’s behavior is simulated with a mesh of computational calculations, as seen in the compacted front end of the car shown. The car is covered with over 1.5 million points, each a separate calculation. (Image courtesy of Livermore Software Technology Corporation.)

acknowledges, “I was very lucky to work at the Laboratory when I did. Software development in house was superior to what was available outside, which motivated me to continue on that path.”

Beyond national security applications, Hallquist realized DYNA3D could be used for any scenario in which materials collide at high speeds. Responding to external requests, the Laboratory released DYNA3D to the open-source community, where the code gained popularity among software developers working on similar impact problems in the automotive, aerospace, and nuclear industries. As interest in DYNA3D increased, Hallquist founded Livermore Software Technology Corporation to develop crash-test software, with emphasis on automotive and aerospace applications. The resulting commercial product, LS-DYNA, has also found a home in manufacturing, consumer products, civil engineering, electronics packaging, and defense. Other applications include





metal stamping, shipping container design, earthquake engineering, and even the simulation of sports equipment and aircraft bird strikes.

For the automotive industry, LS-DYNA has been nothing short of revolutionary. Hallquist's company developed crash simulations to predict vehicle behavior in collisions, reducing the need for expensive tests with real cars. Seatbelts, airbags, accelerometers, and other specialized vehicle components are also designed with the help of LS-DYNA. The industry has seen multibillion-dollar savings over the last three decades, and the Computer History Museum in Mountain View, California, honors Hallquist in its exhibit on crash-test software. Altogether, more than 2,500 companies worldwide have reaped benefits in cost savings and safety advancements with LS-DYNA's stress and deformation prediction capabilities.

Hallquist's code lives on at Livermore as the impact-simulation software PARADYN, which is scaled for massively parallel supercomputers. Among PARADYN's accomplishments is simulating impact response in military helmets to improve helmet padding and reduce traumatic brain injury. Laboratory defense systems engineers use PARADYN for modeling impact events that involve large deformations or debris fields, such as satellite collisions in space, or that occur over subsecond timescales, such as ballistic missile scenarios. (See *S&TR* July/August 2009, pp. 4–11; and *S&TR* September 2012, pp. 26–29.)

## Phase 2: Secure a Network

Martin Casado's journey to entrepreneurship began in high-performance and distributed computing. His simulation work at Livermore shifted focus to cybersecurity in the wake of the September 11, 2001, terrorist attacks. He states, "The Laboratory was my introduction to networking and security." Motivated to solve network vulnerability problems, Casado entered a Stanford University Ph.D. program, where he developed a method to protect networks



Hall of Fame inductee Martin Casado also received the 2012–2013 Grace Murray Hopper Award for Outstanding Young Computer Professional of the Year and has been featured in *Silicon Valley Business Journal*'s "40 Under 40" list, *Business Insider*'s "50 Most Powerful People in Enterprise Tech," and *Forbes Magazine*'s "Next-Gen Innovators." (Photograph by Julie Russell.)

by decoupling software from traditional hardware-centric systems. The network could now be managed by a software application instead of a traditional network and was therefore no longer constrained by or exposed to network security problems.

Software-defined networking (SDN), as Casado's concept came to be called, quickly transformed how the computer industry exchanged data. The paradigm enables microsegmentation, whereby system engineers can configure each application to access only the data needed, not an entire data center. In this way, the modern data center can provide both context—users, data, and files—and isolation, that is, sufficient security control. Casado notes, "SDN architectures can be made more secure than traditional architectures and offer more in-network security services." SDN technology is flexible and responsive and reduces the time and cost of provisioning and scaling a virtual network.

While at Stanford, Casado founded Illuminics Systems, an Internet protocol analytics company, and helped develop code for the network platforms OpenFlow and Open vSwitch, expanding SDN technology into the open-source community. A new market was thus born, along with Casado's second startup company, Nicira Networks, to develop SDN applications. Casado says, "My job at the Laboratory was the most formative job I've ever held and laid the foundation for my subsequent work."

In 2012, Casado sold Nicira Networks for \$1.26 billion. Now a general partner at Andreessen Horowitz, he focuses on software infrastructure investments and works closely with the founders of companies in the portfolio. Healthcare, banking, and retail are just a few industries reaping the benefits of SDN. Casado explains, "Because this technology allows automation of network infrastructure and provides security services within a data center, it solves a lot of 'sticky' problems that come with computer virtualization, such as providing strong isolation and the mobility of security policies."

## Phase 3: Achieve Liftoff

Laser physicist Brent Dane and physicist Lloyd Hackel combined their complementary backgrounds to achieve a manufacturing breakthrough. Hackel remembers, "Our group at the Laboratory had been developing laser technology for x-ray lithography to print computer chips and for space object imaging. We then realized that our laser was ideal for laser peening." Dane and Hackel eventually partnered with Metal Improvement Company, Inc., to evolve an advanced method of laser peening. Livermore's IPO brokered a CRADA for a commercial system, and both scientists eventually transitioned to Metal Improvement Company, which today is part of Curtiss-Wright Surface Technologies.

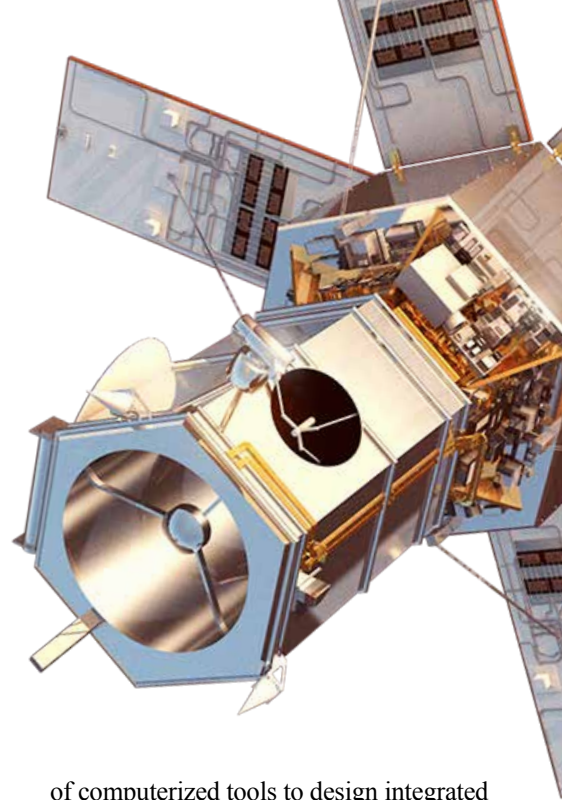
Laser peening, in which laser beams replace traditional metal shot, involves

firing a series of intense laser blasts at a surface. By producing a shockwave that creates a compressive stress field in the surface, the lasers strengthen the underlying material. Dane and Hackel pioneered a high-energy laser with increased pulse frequency, beam imaging, and robotic controls that enable components and systems to run longer and with greater safety margins. Their package of technologies became marketed under the name Lasershot Peening System. Dane notes, “Our work increases the fatigue strength of metal components by preventing the initiation and growth of cracks.” The result is life extension for critical parts subject to intense conditions, such as aircraft fuselages and turbine blades used in jet engines and electric power generation. (See *S&TR*, March 2001, pp. 26–28.)

The team also developed a peening process to plastically strain materials to form precision curvatures in thick or complex components. Hackel explains, “We patented the concept of shaping metals with laser peening and preferentially controlled shaping with prestressing techniques.” The process is most notably applied to workpieces over 100 feet long. Since 2008, the Boeing Company has used the Lasershot Peening System to manufacture wing panels for 747-8 aircraft. Dane adds, “We have a rapidly growing presence in defense applications where the use of laser peening has moved from engine components to airframes.” Today, jet engines and aircraft wings run more efficiently and cost-effectively because of the team’s innovations.

Lloyd Hackel (left) and Brent Dane stand with a robot used in laser peening to strengthen critical parts for aviation and other industries. The duo successfully commercialized a laser peening technology—marketed as the Lasershot Peening System—used around the world in airplane fuselages and turbines, as well as in turbines for electric power generation. (Photograph by Julie Russell.)

Walter Scott helped found the company known today as DigitalGlobe, which most notably provides satellite imaging content for Google Maps. The company’s satellites collect more than 4 million square kilometers of Earth imagery every day at industry-leading resolution, geopositional accuracy, and spectral diversity. The imaging technology’s many applications include enabling relief agencies to reach people in need after a natural disaster, allowing companies to monitor global infrastructure, and helping humanitarian organizations expose human rights abuses. (Image courtesy of DigitalGlobe.)



Additional metalworking products that benefit from the technology include arrestment hook shanks used for carrier-based aircraft and ship-propulsion shafts currently under development. A new mobile laser peening system rapidly delivers the process to remote locations, and in 2016, Metal Improvement Company successfully treated 110-ton steel pieces at a customer worksite. Hackel states, “We’re also preventing stress corrosion cracking in containers for spent nuclear fuel.”

### Phase 4: Change Perspectives

Computer scientist Walter Scott joined the Laboratory in 1986. His development

of computerized tools to design integrated circuits led to involvement in the Department of Defense’s Strategic Defense Initiative. He then became leader of the Brilliant Pebbles Program, which aimed to stop ballistic missiles with small spacecraft. Scott notes, “Livermore is an incredibly exciting environment for a technologist, with opportunities to work on very hard problems of high national importance. Both aspects were strongly motivating.” The work gave him insight into emerging trends in satellite technology, which was becoming more affordable thanks to microelectronic innovations, as well as advances in the graphics capabilities of personal computers.







The geopolitical landscape was changing, too. Scott describes his “ringside seat to the end of the Cold War” as a formative experience. He says, “This fluid environment created an opportunity to use satellite imagery to provide global transparency to a much broader set of users.” In 1992, Scott founded Colorado-based WorldView Imaging Corporation, which became the first company to strike a satellite-imaging deal with the U.S. government. Now named DigitalGlobe, Scott’s company has launched a host of high-resolution imaging satellites, has amassed a 100-petabyte time-lapse image library, and most notably provides satellite imaging content for Google Maps and many other online mapping sites.

Early collaboration with John Henke, cofounder of the data visualization software company Keyhole, led to the industry’s highest-resolution satellite imagery. Scott notes, “Google needed the data from our QuickBird satellite to build a world-class mapping application. After a meeting with [Google founders] Sergey Brin and Larry Page, we had a deal.” DigitalGlobe’s continued deployment of advanced technologies aboard commercial imaging satellites includes high-fidelity sensors that detect parts of the electromagnetic spectrum beyond human visibility. The company has created the most comprehensive geospatial ecosystem featuring a big-data platform, global distribution channels, and a



The Lasershot Peening System has improved the fatigue life of jet engine and turbine components for a roster of high-profile commercial planes, such as Airbus’s A340 and A350, Boeing’s 777 and 787 Dreamliner, and Gulfstream’s G650. The technology is also used in military aircraft, including the F-22 Raptor and F-15 Eagle. Ongoing development will expand this use to the A-10 Thunderbolt, C-17 Globemaster, and F-35 Lightning models B and C (B shown here). (Image courtesy of U.S. Navy.)

growing repository of analytic tools. Now heading into a \$2.4-billion acquisition, DigitalGlobe’s geospatial analysis and satellite imaging technologies are poised for new applications with help from machine learning, elastic cloud computing, and crowdsourcing. Scott notes, “Combined, these tools unlock the rich information in our image library to create applications previously impossible, such as monitoring economic activity from space, developing continent-wide property databases for the insurance industry, enabling safe drone navigation, and supercharging the effectiveness of overworked intelligence analysts by narrowing the search space.”

### Investment in the Future

Surrounded by modern technology and with access to resources and equipment for experimentation, Livermore scientists solve complex problems every day. Rankin sees commercial potential in many growing research areas across the Laboratory. He notes, “We can make significant contributions in additive manufacturing and next-generation energy technology. Biomedical engineers are designing devices and processes that directly impact our quality of life.” He cites as examples the three-dimensional printing of blood vessels (see *S&TR*, March 2016, pp. 13–16) and work under the National Institutes of Health’s Brain Research through Advancing Innovative Neurotechnologies (BRAIN) Initiative.

Hall of Fame members also recognize the invaluable asset that IPO represents to Livermore scientists trying to convert their technology into a commercially viable product. Hackel says, “The Laboratory was a tremendous place to advance my knowledge and further my experimental and project management capabilities. IPO was especially helpful with patenting, agreements, and other legal support.” Scott also acknowledges IPO’s support, stating, “The Laboratory was willing to review intellectual property and give me clear guidelines, allowing me to continue my work while raising the financing to get DigitalGlobe off the ground.” These achievements in technology transfer indicate how this mission of IPO’s is a natural extension of Livermore’s mission in national security. Rankin says, “The Laboratory is an exciting place behind the fences. We want the public to understand that the Department of Energy’s technology base makes a positive impact on their lives in so many ways.”

—Holly Auten

**Key Words:** commercialization, cybersecurity, DYNA3D, Entrepreneurs’ Hall of Fame (EHF), entrepreneurship, geospatial analysis, Industrial Partnerships Office (IPO), laser peening, Lasershot Peening System, LS-DYNA, PARADYN, satellite imaging, software-defined networking (SDN), technology transfer.

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# From the Laboratory to the **WORLD**



**T**HE pathway from national laboratory to marketplace is often impeded by barriers that can prevent Laboratory technologies from meeting their full commercial potential and benefiting as many people as otherwise possible. Barriers can include the time and expense associated with identifying a market need for a technology, scaling up the technology to meet that need, building a business-savvy team of scientists to groom the technology into a marketable product, and finding investors to help make the plan a reality. To overcome these obstacles and accelerate the transfer of national laboratory science from the workbench to the marketplace, Lawrence Livermore's Industrial Partnerships Office (IPO) and the Department of Energy (DOE) provide valuable guidance and resources to educate Laboratory scientists and engineers about business and commercialization.

One resource is DOE's Energy I-Corps (formerly known as Lab-Corps). This program, which aims to accelerate the commercialization of clean-energy technologies, is a rigorous eight-week multilaboratory entrepreneurial "boot camp" where participants dig deep into the nuts and bolts of real-world technology transfer. A team entering the program consists of at least one technical expert, an entrepreneurial lead, and an industry mentor. All participate in a variety of activities designed to advance entrepreneurial knowledge and map out potential paths to commercialization.

Six Livermore teams have participated in Energy I-Corps since its inception in 2014. Yongqin Jiao is the principal investigator of MicroMiners, a project focused on rare-earth bioadsorption, that is, using genetically engineered bacteria to recover rare-earth



elements from sources, such as waste, where levels are so low that recovery by ordinary means would be prohibitively expensive. The rare earths are critical for many U.S. industries, including clean energy, and for national-security applications such as optics at the National Ignition Facility. (See *S&TR*, April/May 2016, pp. 17–20.) Jiao says, “Before we participated in Energy I-Corps, our team did not have the knowledge to successfully transfer our rare-earth recovery technology to industry.” The program connected the team to their potential market and even helped them attract funding to better adapt their technology to market needs. In fact, this deeper understanding of the marketplace inspired a shift in their approach to the research. Jiao explains, “Now, when we work in the laboratory, we think of our research in the context of prospective industry applications. This change in perspective bolsters our drive to work more rigorously to push our technology out to the market so it can begin to make a real impact.”

### Captivating a Customer

Customer discovery represents a major element of Energy I-Corps. During this step, participants are challenged to interview at least 100 potential customers, an experience that helps identify not just a specific application but also specific customers. Sometimes scientists find that their technology will fulfill a different need than originally envisioned. Postdoctoral engineer Congwang Ye and his team designed silicone microcapsules that can capture carbon dioxide ( $\text{CO}_2$ ) from waste gas more safely, quickly, and affordably than other techniques. (See *S&TR*,

December 2015, pp. 13–16.) Although the technology was originally targeted for power plants, Energy I-Corps helped Ye’s team find an industry application in breweries. The fermentation process that produces alcohol also generates  $\text{CO}_2$ , which is normally released into the atmosphere. Captured  $\text{CO}_2$  could be reused later to carbonate the beer, instead of purchasing  $\text{CO}_2$  as breweries typically do. Ye’s team proposed providing breweries a  $\text{CO}_2$ -capturing system comprising a tank filled with millions of the microcapsules to absorb  $\text{CO}_2$  from the fermentation gas. When the tank is saturated with gas, the team would collect and replace it. The reclaimed  $\text{CO}_2$  could be sold back to participating breweries or other nearby users. Because the current capsule was designed for a different gas composition than brewery fermentation gas, the team will continue their research to adjust the microcapsule design accordingly. The team is in discussions with the University of California (UC) at Davis to validate the system at the university’s pilot-scale brewery.

Without Energy I-Corps, Ye admits he would not have thought about applying his technology to the beer industry. Like Jiao, he learned through the program to think about the practical applications of technology in the marketplace, the importance of

Members of multiple Energy I-Corps teams, faculty, organizers, and Department of Energy personnel attend the graduation of the program’s fourth cohort in Denver, Colorado, in December 2016. (Photograph courtesy of the National Renewable Energy Laboratory.)

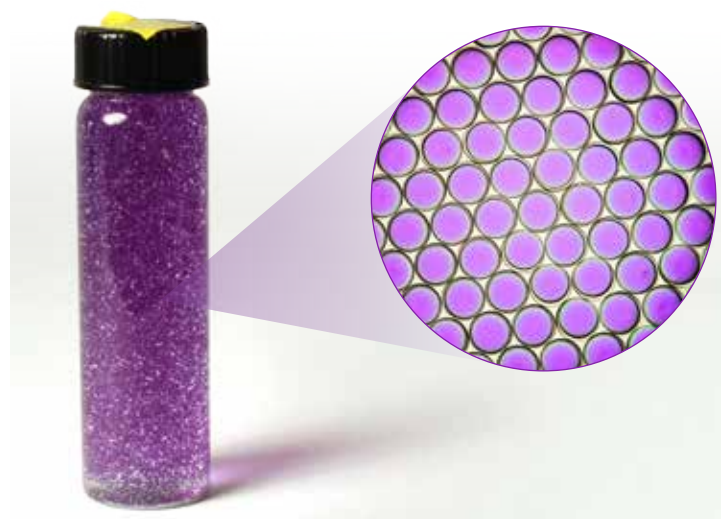


communicating with potential customers, and how to collaborate with seasoned mentors to come up with a successful business plan. Hannah Farquar, Livermore's Energy I-Corps liaison, says, "Our participants come to realize they are no longer addressing a problem unique to national security. Instead, they're using advanced Laboratory capabilities and expertise to provide a solution to a real market challenge."

### Accelerating Advancements

Seeking to expand on the success of Energy I-Corps, DOE issued a call to the national laboratories for ideas. IPO proposed a broader and more ambitious business education system based on one already in place at Livermore. Similar to a business school, the system trains budding entrepreneurs in relevant business skills, including market research, customer discovery, and product development. Roger Werne, IPO's deputy director, says, "Through this system, scientists and engineers come to understand more about industry and are therefore more likely to find a successful match for their technology in the outside world." DOE eventually decided to expand the Livermore approach to all DOE laboratories. The new, larger program is dubbed the National Laboratory Accelerator Program.

Participants in the National Laboratory Accelerator Program first attend the National Laboratory Entrepreneurship Academy, a three-day course at UC Davis that drills participants in basics such



Silicone microcapsules contain a sodium carbonate solution that traps CO<sub>2</sub>. Although originally designed to capture CO<sub>2</sub> from flue gas, the capsules could also be used by breweries to capture CO<sub>2</sub> released as part of the fermentation process.



Livermore researcher Congwang Ye (left) visits with professors at the University of California at Davis at their pilot-scale brewery to learn about fermentation tank operations as part of his adaption of a microcapsule technique for trapping carbon dioxide (CO<sub>2</sub>) to commercial breweries. Ye hit on this application through his participation in Energy I-Corps.

as business model, value proposition, and customer discovery. A firm grasp of these steps allows scientists and engineers to better develop, analyze, and validate the commercial potential of their work. They also learn how to communicate with the business world, becoming familiar with industry terminology and learning to rely less on technical language. Werne states, "Our scientists and engineers are comfortable explaining how their technology works to colleagues and sponsors, but the key to success in this process, rather, is clearly communicating what their technology can do for industry."

After this initial training, each budding entrepreneur pairs with an experienced non-Laboratory business mentor who aids in further developing the initial concept. This collaboration steers the concept's maturation while fostering a close working relationship with the entrepreneurial community—important for establishing connections with related markets and potential partners. In some circumstances, the mentor may see great potential in a protégé's technology and become even more involved in the project, even to the point of becoming a partner or investor.

The rare-earth element extraction technology developed by Jiao greatly interested Jim Kiles, Jiao's industry-savvy mentor. Kiles is founder and chief executive officer of Ystrategies Corporation, a business development and venture capital firm that invests



## Accelerating Innovation

Hybrid-electric vehicles, fluorescent lights, large wind turbines, and other clean-energy products all rely on small quantities of rare-earth elements. However, these elements are often expensive, with demand exceeding supply because of the difficulty of extraction with conventional methods. The combination of scarcity and high cost creates an urgent need for new approaches to efficiently and cleanly recover these materials from ores and recyclable products.

Livermore staff scientist Yongqin Jiao and colleagues are leading a project to develop an environmentally friendly bioadsorption strategy for rare-earth recovery using a genetically engineered bacterium. Attached to the bacterium's outer cell wall are lanthanide-binding ligands, which attract rare-earth atoms with 1,000 times greater affinity than for other metals. Rare earths adsorbed by the bacteria can be washed off with a solution of citrate, a derivative of citric acid that is harmless to the bacteria, allowing the organisms to be reused many times. Applications originally envisioned for this novel technique include the processing of low-grade waste materials such as mine tailings, coal byproducts, and geothermal brines.

Jiao's team participated in the Department of Energy's Energy I-Corps program to further develop their technique for the U.S. clean-energy industry. Through the program, the team identified geothermal and coal mining companies interested in adopting the technology. The Livermore team and the companies are now working together to

commercialize the technology and thereby supply the nation with a more secure source of the important materials.



Livermore's Yongqin Jiao (left) and Suzanne Singer, members of the MicroMiners team for rare-earth recovery, engage with industry expert Tim Heaton as part of the Department of Energy's Energy I-Corps program. The program pairs national laboratory researchers with industry professionals who can help enhance a technology's commercial potential.

in advanced clean-energy technologies designed to minimize disruption to business processes. Clean-energy technologies using rare earths fit that bill but lacked market appeal because of the elements' costs. (See box above.) Kiles explains, "Because of the scarcity of rare-earth elements, the demanding market for the materials is suffering. However, this Livermore extraction technology can potentially solve a major industry issue and propel the success of related businesses."

The next step in the National Laboratory Accelerator Program is for the scientists, engineers, and their mentors to participate in Energy I-Corps or a similar program for intensively studying customer discovery, product-market fit, and business model development. After this step, some participants continue working until their business concept is deemed ready to unveil to investors. Those whose technologies demonstrate exceptional potential are invited to a competition where the most promising team from each of the 10 participating national laboratories pitches their technology to actual investors ready to offer seed funding to the right team.

Access to the advanced technologies and intellectual property of a national laboratory helps industry partners to develop products with the potential to improve society. In return,

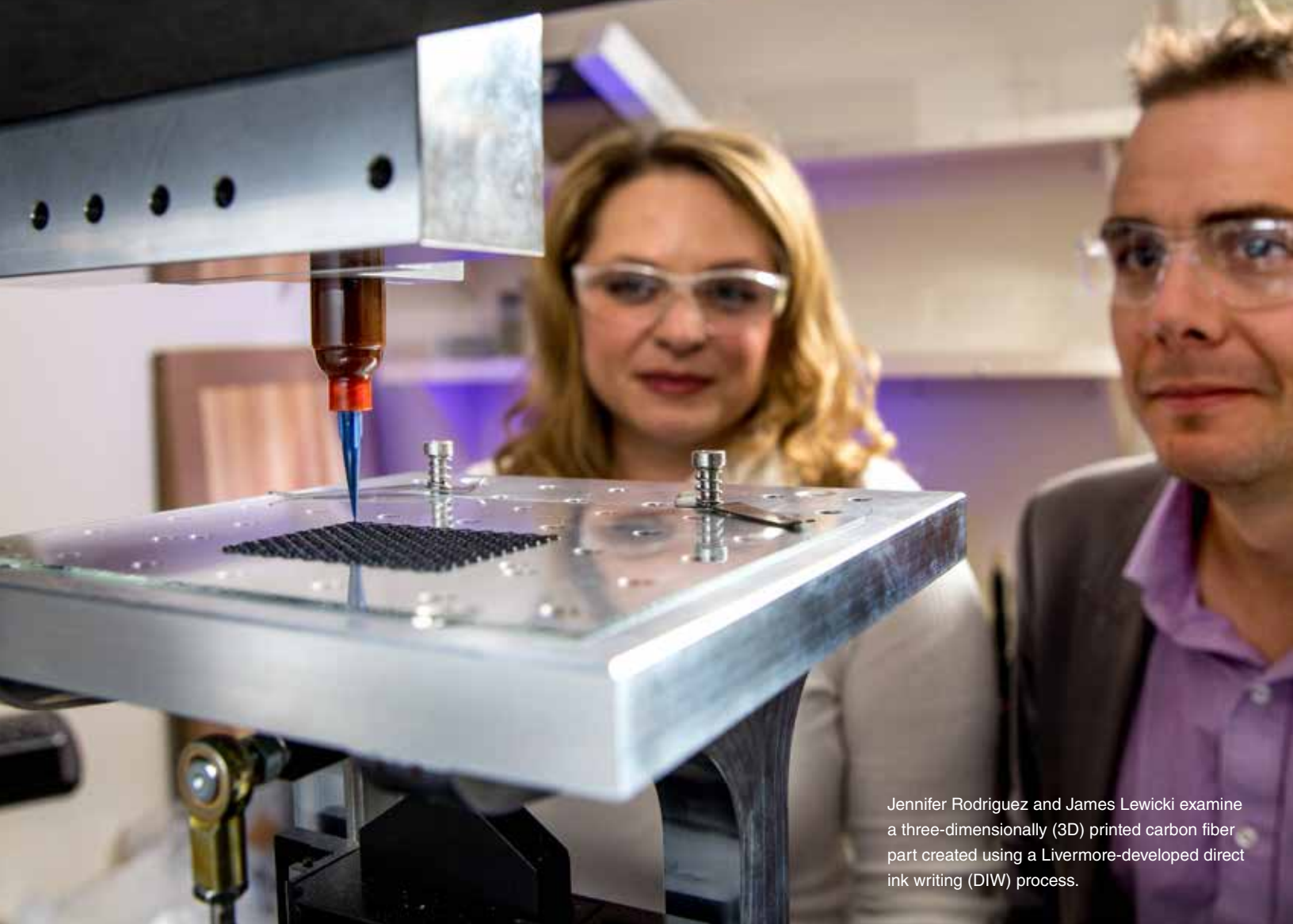
these partnerships help the national laboratories develop and sustain the very capabilities that further their national security mission. Energy I-Corps and the rest of the National Laboratory Accelerator Program promote this mutually beneficial partnership, combining the expertise and resources of the national laboratories, collaborating universities, and business partners to accelerate the commercialization of promising national laboratory technologies. The successes already achieved demonstrate that these public-private collaborations add value to both the national laboratories and the nation's economy. Werne states, "The question is, can we boost the nation's economic competitiveness? We can. We do. We have."

—Lanie L. Helms

**Key Words:** carbon capture, carbon dioxide (CO<sub>2</sub>), clean-energy technology, commercialization, Energy I-Corps, Industrial Partnerships Office (IPO), MicroMiners, National Laboratory Accelerator Program, rare-earth elements, technology transfer.

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# A NEW COMPOSITE-MANUFACTURING Approach Takes Shape

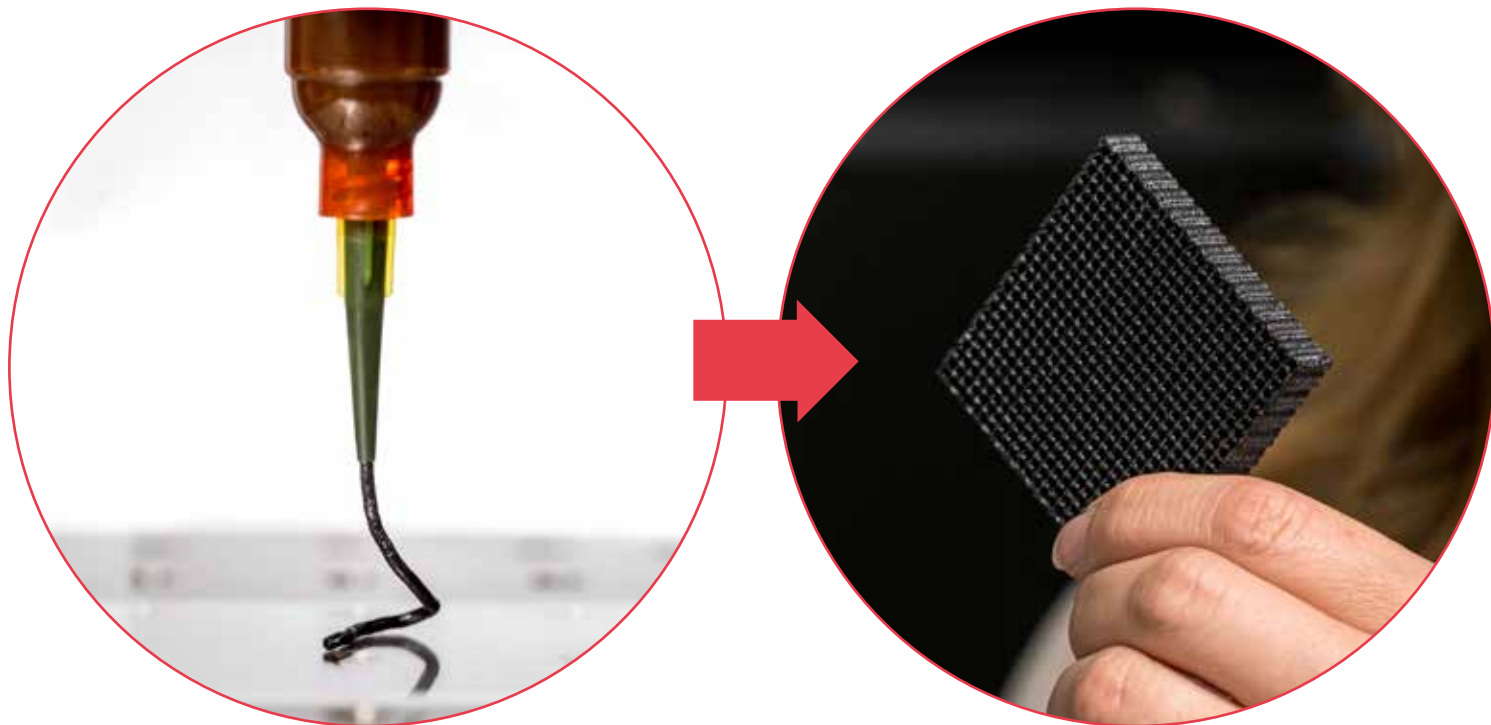


Jennifer Rodriguez and James Lewicki examine a three-dimensionally (3D) printed carbon fiber part created using a Livermore-developed direct ink writing (DIW) process.

**S**TRONGER than steel yet lightweight as plastic, electrically conductive and highly temperature resistant, carbon fiber composites have become the material of choice for many applications in aerospace, transportation, defense (see *S&TR*,

March 2013, pp. 4–9), and energy storage. The heterogeneous nature of these mixtures of carbon fibers and resin allows for greater customization of structure and properties than with more homogenous materials, such as steel. However, the materials





also pose significant manufacturing challenges. For instance, variability within and between parts can be greater than with homogeneous materials, and such variations can affect a part's properties and performance, which depend heavily on fiber orientation and distribution. Fabricators can compensate for this variability with a higher ratio of fiber to resin, but doing so makes the parts heavier and costlier and the process more wasteful than necessary.

Additive manufacturing (AM)—commonly known as three-dimensional (3D) printing—could eliminate many of these manufacturing concerns. By depositing a material layer by layer in a precise sequence specified in a computer file, AM enables greater precision, design flexibility, and repeatability than conventional manufacturing techniques. Plastic and metal AM technologies are well established, but printing carbon fiber composites is a tangle that scientists and engineers have only begun to unravel over the past few years.

Livermore chemist James Lewicki says, “Carbon fiber is the ultimate structural material. If we could make everything out of carbon fiber, we probably would, but it’s been waiting in the wings for years because it’s so difficult to make in complex shapes. With 3D printing, however, we could potentially make any shape.” Lewicki leads a team of chemists, engineers, materials scientists, and computational experts who—with

In DIW, a type of additive manufacturing, (left) a tiny nozzle extrudes a liquid combining carbon fiber and polymer resin onto a platform in a pattern prescribed by a computer file. Layer by layer, as the 3D structure is built, the “ink” must extrude smoothly and solidify quickly to support the growing structure. (right) A completed 3D-printed part is shown.

funding from the Laboratory Directed Research and Development Program—are working to improve the versatility and predictability of carbon fiber 3D printing and the performance of the resulting parts. Combining computational modeling and novel materials chemistry with AM techniques, the team has successfully demonstrated a new approach to producing high-performance carbon fiber composites.

### A Better Glue

Carbon fiber composites are made of fibers just 5 to 10 micrometers in diameter, set in a polymer matrix known as a resin. The carbon fibers provide most of the material's strength and other performance characteristics. The resin binds the fibers together to prevent buckling but also represents one of the biggest obstacles to the 3D printing of high-performance parts using direct ink writing

(DIW). DIW is a high-speed, low-cost AM technique in which “ink”—a material in liquid form—is extruded through a tiny nozzle and onto a platform that is moved to deposit the ink where needed to build up the desired object, layer by layer, in three dimensions. (See *S&TR*, March 2012, pp. 14–20.) With DIW, manufacturers can print a wider variety of structures, geometries, and patterns than with conventional approaches, but existing DIW resins are not strong enough for high-performance applications such as aerospace. Nor are most high-performance resins suitable in another important regard—curing time. Conventional resins can take hours or days to harden, while the DIW process requires a resin that can hold its shape as the component is built up. Furthermore, most conventional composites would clog the nozzle of a DIW printer rather than extrude smoothly and continuously.

With no commercially available resin to meet their needs, Lewicki and his team created a resin specifically for high-performance component printing—one that gels in 5 seconds or less, fully cures with heat in 10 minutes, and offers flow characteristics suitable for AM. A low volume of high-surface-area silica nanoparticles yields an optimal resin consistency and allows the carbon fibers to orient themselves in the direction of the flow as they are squeezed through the nozzle, preventing clogging.

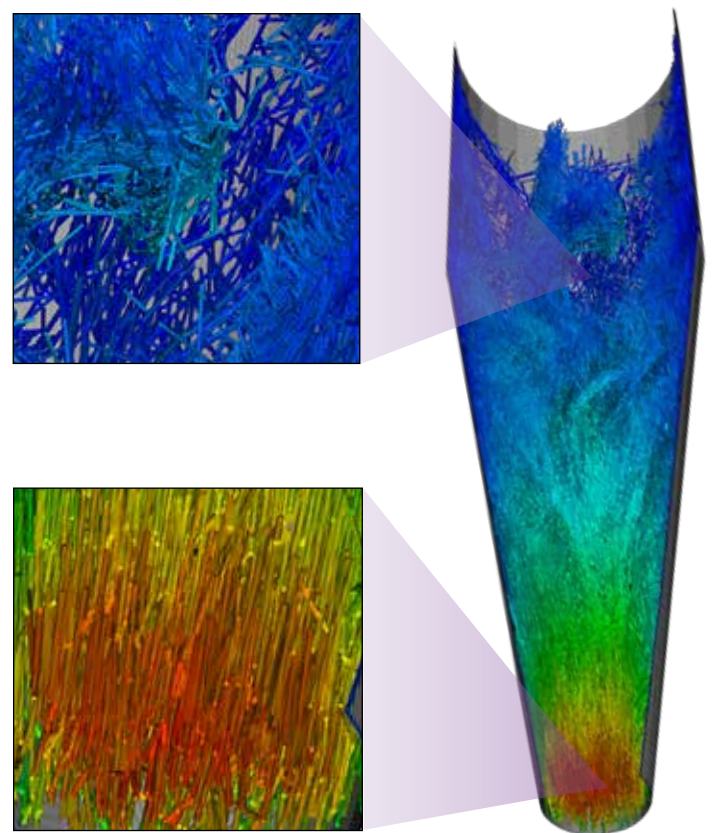
The resin formula is as much a product of computer simulation as innovative chemistry. In developing the resin, the team’s computational experts used Livermore supercomputers to model the flow of carbon fibers through the ink nozzle at several scales. Lewicki notes, “Simulations of the actual printing process were important early on, as they helped show us the path forward with fewer experimental iterations.” Fluid analyst Yuliya Kanarska adds, “With our code, we can simulate the evolution of the fiber orientations in 3D under different printing conditions to find the optimal fiber length and optimal performance.” Simulation results both validated and explained what was observed experimentally—that with the right ingredients in the right ratio and the right nozzle size and shape, the resin can efficiently deliver carbon fibers without clogging the printer.

### Designer Parts

Standard mold-based manufacturing methods and even some other DIW formulations produce parts with a more random fiber distribution and alignment than Livermore’s approach does. Livermore parts, with fibers more consistently aligned in the flow direction, have superior mechanical properties compared to those with the same density of fibers produced by other methods. Recognizing this advantage, the team has gradually increased the

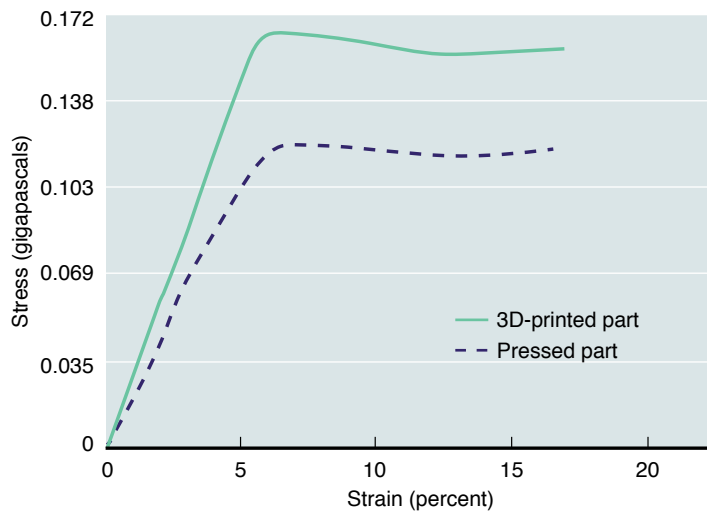
volume of carbon fiber in their formula and can now create parts with the same level of performance as traditionally manufactured parts but with just one-third the carbon fiber volume that would be required by other carbon fiber composites. Engineer Michael King states, “We are now confident we can design parts that perform better on a per-fiber and an overall-part basis than other methods can.”

Precise yet flexible, DIW offers researchers the freedom—and challenge—of tailoring a part’s electrical, mechanical, and thermal response to a given application. Lewicki says, “With chemistry



To avoid nozzle clogging in DIW printing, Livermore researchers use high-resolution numerical simulations of carbon fiber “ink” to study the evolution of fiber orientations in three dimensions. The simulations, such as the one shown here, have helped researchers understand the relationship between fiber length, nozzle diameter, and degree of fiber alignment relative to flow direction. Colors reflect degree of alignment, with warmer colors indicating greater levels of alignment than cooler colors. Fibers approaching the nozzle at bottom start to orient with the direction of flow.





In mechanical testing, 3D-printed parts made with the Laboratory's carbon fiber composite—in which fibers are oriented in the printing direction—outperform conventional pressed parts, which contain randomly aligned fibers.

and engineering, we can purposely put carbon fiber exactly where we want it in a part, more so than other research groups can do. But then the question is, where *should* we put the material for the best performance?" For example, satellite components could be printed to be insulated on one side and conductive on the other to compensate for heat-induced warping.

Because no existing composite-design algorithms could satisfactorily optimize performance, the team has been writing their own, building on team and institutional expertise in multiscale material modeling and systems optimization. Subsequent efforts to optimize fiber layout for greater strength and stiffness in certain directions yielded a 15 percent improvement in mechanical properties, with the potential for even greater improvements.

Computational optimization is an essential step towards making carbon fiber 3D printing predictable, repeatable, and highly customizable. Although still in its infancy, this effort aims to integrate process modeling and computational optimization with in-house tool-path planning algorithms, for a workflow of robust, computationally aided design, development, and manufacturing. The tool-path planning currently under way will assess a part's optimized design, confirm that the design is printable, and then translate the design parameters into instructions that the 3D printer understands. King says, "Essentially, we are building thousands of parts virtually to produce optimized machine instructions, so that we can

ultimately get a highly buildable part." To this end, the team continues to investigate the structure and properties of the composite ink when used in DIW manufacturing. Characterization and modeling aim to better understand and control the properties and performance of the resulting AM structures.

### From Idea to Product

With enhanced design flexibility, manufacturing repeatability, and part performance, AM technology is expected to spur wider adoption of the team's versatile carbon composite. Lewicki has been working with Genaro Mempin in the Laboratory's Industrial Partnerships Office to develop a commercialization strategy, including filing records of invention (ROIs)—the first formal step on the path to a patent. The ROIs expand Livermore's already sizable portfolio of AM-related innovations, underscoring the institution's core competency in advanced materials and manufacturing. Mempin says, "We have received more than 90 ROIs in AM from Livermore inventors since 2009. The Laboratory has filed patent applications for more than two-thirds of these ROIs, and more are in the pipeline being prepared to file."

Lewicki notes, "So many people are interested in a better, faster, cheaper way to make carbon fiber composites. To take this project further, however, we need to make the transition from scientifically interesting material to practical industrial product. For this, we need collaboration." The research team is exploring a range of opportunities. Other Livermore teams engaged in national and energy security research, along with potential U.S. defense partners and potential licensees in commercial aerospace, have already expressed an interest in Livermore's resin formulation and AM process optimization.

The secret formula behind the team's innovations, according to King, is actually quite simple: "We have a tight collaboration between computational experts, chemists, and engineers. Multidisciplinary teams are something the Laboratory does well and are what has allowed us to create a practical, high-quality technology."

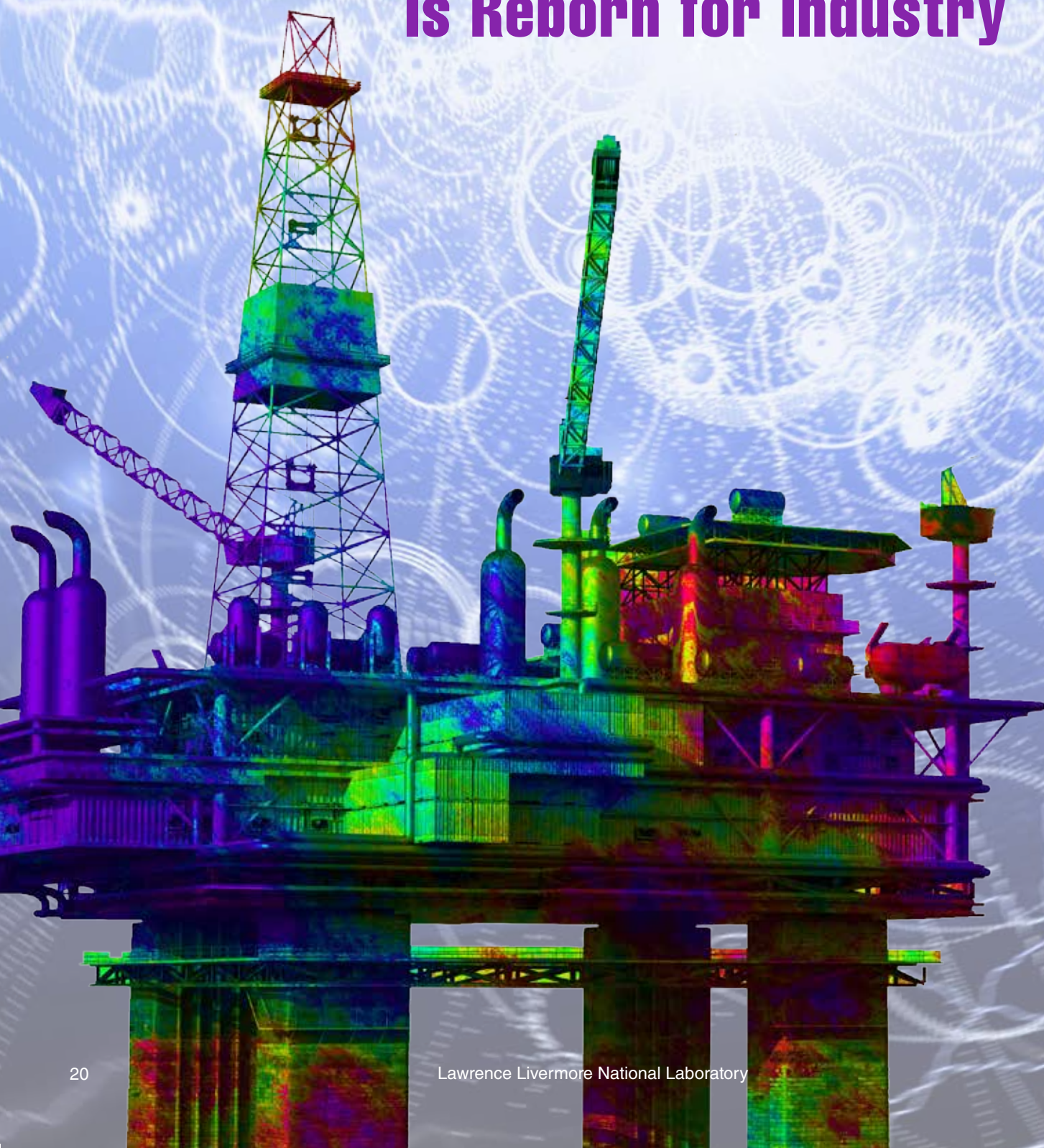
—Rose Hansen

**Key Words:** additive manufacturing (AM), carbon fiber composite, design optimization, direct ink writing (DIW), Industrial Partnerships Office, Laboratory Directed Research and Development Program, record of invention (ROI), resin, silica nanoparticle, three-dimensional (3D) printing, tool-path planning.

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# A National Security Code Is Reborn for Industry





**F**OR decades, Lawrence Livermore researchers have developed simulation codes that run on some of the world's most powerful supercomputers. These codes predict how materials and systems will perform in a variety of environments, including extreme conditions of temperature and pressure. Livermore's far-reaching predictive capability through simulations is particularly important for national-security efforts such as stockpile stewardship, the National Nuclear Security Administration's program to ensure the safety and reliability of the nation's nuclear stockpile.

A highly versatile and popular Livermore code is ALE3D, whose name refers to arbitrary Lagrangian–Eulerian three-dimensional (3D) analysis. First developed nearly 30 years ago, ALE3D is a multiphysics software tool used by researchers nationwide to solve various engineering and physics problems important to national security. Since its creation, ALE3D has been limited to U.S. citizens working on mission-relevant applications at Lawrence Livermore and other national laboratories, as well as the departments of Energy, Defense, and Homeland Security and their contractors. This limitation has inhibited the Laboratory from partnering with nondefense industries and universities to solve many other challenging problems using ALE3D.

Now, a team led by Livermore computational engineer Chad Noble is developing a version of ALE3D called ALE3D-4I (“ALE3D for Industry”) that can be widely shared with research partners interested in a much broader range of applications. The new code will be available for use on the Laboratory's massively parallel supercomputers—machines with tens of thousands of processors working in tandem. U.S. companies and academics interested in using the code and Livermore's high-performance computing (HPC) resources will be able to do so through the

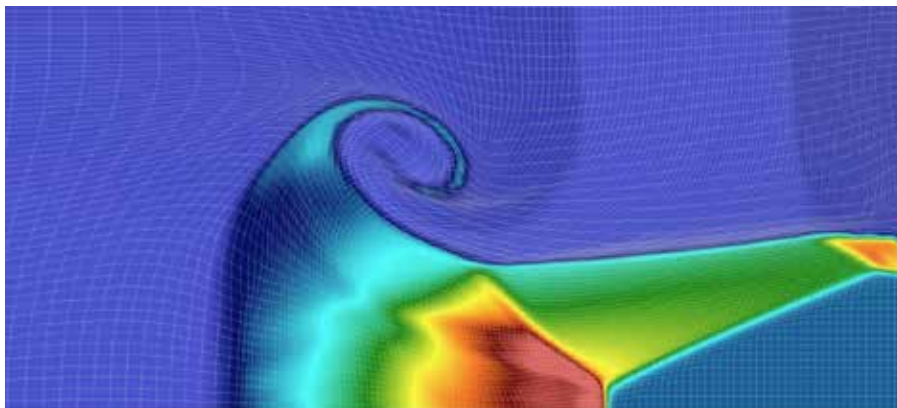
Laboratory's High Performance Computing Innovation Center (HPCIC). (See *S&TR*, March 2015, pp. 4–10.)

ALE3D-4I is the culmination of an effort launched in 2016 with the allocation of special funds to Noble's team. The funds, called innovation development funds, are administered by Livermore's Industrial Partnerships Office and come from the licensing and royalty fees that the Laboratory earns from Livermore-developed technologies transferred to industry. The initial version of ALE3D-4I, expected to debut in the summer of 2017, will feature a subset of ALE3D capabilities relevant to potential industrial and academic partners.

### Expanding Collaborations

Developing ALE3D-4I and making the code available to industrial and academic partners will not only provide new, unmatched capabilities to these partners but also further the Laboratory's missions by making existing algorithms more robust through application across a broader spectrum of uses. The effort also provides potential funding to develop new capabilities of interest to both industry and program sponsors and promote growth of the code team, resulting in deeper expertise across the project.

As the “ALE3D for Industry” name implies, a principal goal of ALE3D-4I is to provide industry a unique advanced computer simulation tool for improving the nation's economic competitiveness. “U.S. industry is looking for a competitive edge by leveraging HPC,” Noble explains. He notes that ALE3D's capabilities and name recognition, coupled with Livermore's longstanding know-how in software quality assurance and code verification and validation, make the code highly sought after by the private sector. Although several commercial and open-source codes similar to ALE3D-4I are



Lawrence Livermore's ALE3D code is a versatile multiphysics simulation tool used nationwide to solve two-dimensional (2D) and three-dimensional (3D) engineering and physics problems. As with similar programs, ALE3D divides an object into a meshlike assemblage of simple elements. These elements are the units on which the computer calculates the object's changing behavior. However, ALE3D has the ability to “relax” the mesh and force more elements into a specific area of interest, for greater accuracy at that spot. In this simulation of a shocked material, the mesh is relaxed around the area of greatest interest to the researchers.

available, these codes have yet to offer multiphysics capabilities coupled with the ability to run on powerful supercomputers. The Livermore code will fill that market gap by providing both capabilities, together with ready access to other Livermore resources at the HPCIC.

Noble and other Livermore representatives have been holding discussions with potential industrial partners who are interested in using ALE3D-4I to make their operations more productive and their products more cost-effective, for a greater edge in the highly cost-driven global marketplace. Potential applications include the advanced manufacturing of high-technology components, home care products, and food processing and safety. The rapidly growing industry of additive manufacturing—also known as 3D printing—is also keen to conduct simulations modeling possible breakthrough technologies. Basic agreements with industrial collaborators will provide access to the code, as well as to Livermore supercomputers and user support. Furthermore, additional capabilities can be developed for an additional fee.

Universities are also interested in using and extending the capabilities of ALE3D-4I, such as developing advanced algorithms and modeling turbulence and other complex physics. Joint research with universities is expected to propel scientific discovery and also create a hiring pipeline through which the Laboratory can find talented computational scientists and engineers. Lawrence Livermore offers week-long training courses three times a year for new users, and Noble sees both industry and university personnel coming to the Laboratory for training. He says, “We want to make it easy for the new user.”

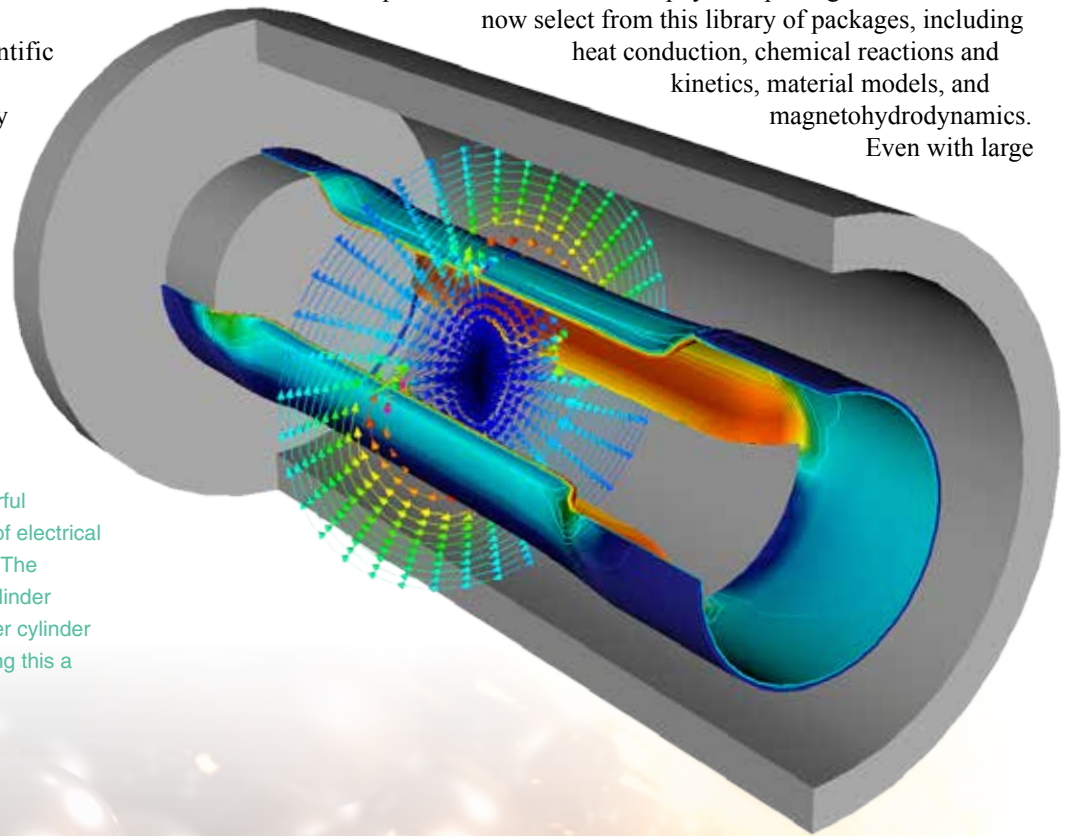
The ALE3D simulation shown depicts powerful magnetic fields generated by a large pulse of electrical current running through an outer conductor. The magnetic fields crush a thin-walled metal cylinder located inside the larger conductor. The inner cylinder is slotted to break the axial symmetry, making this a fully 3D problem.

### How ALE3D Works

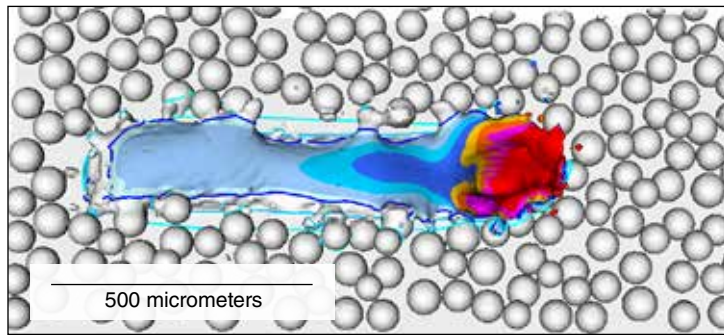
ALE3D’s hydrodynamics capability captures the behavior of both solids and fluids. The code has been successfully used for applications involving long (implicit) and short (explicit) timescales and both two-dimensional (2D) and 3D simulations. Providing 2D capability enhances flexibility, because a user might opt for 2D when 3D would be either too computationally demanding or simply unnecessary, such as when simulating a cylindrical object or another problem involving a symmetrical axis. The code employs finite-element analysis, a method for analyzing engineering problems in which an object is divided into a meshlike assemblage of simple elements. These elements are the units on which the computer calculates the larger object’s changing behavior. Lines forming the element boundaries intersect at junctions called nodes, which define the elements’ movement and deformation. Each node can move in any direction, depending on the stresses and strains applied.

ALE3D began as a hydrodynamics and structure-deformation code to model the behavior of solids and fluids undergoing shock-induced deformation and high strain rates. Over the years, developers added multiphysics capabilities representing various phenomena in the form of physics “packages.” Users can

now select from this library of packages, including heat conduction, chemical reactions and kinetics, material models, and magnetohydrodynamics. Even with large







A newly developed commercial version of ALE3D called ALE3D-4I (“ALE3D for Industry”) enables simulations relevant to U.S. industry. In the case of laser-based additive manufacturing, the simulations precisely predict the characteristics of a metal powder melted by a laser. This simulation depicts heat from the laser moving from left to right, melting and fusing the powder particles. The colors represent different temperatures, with blue being the coldest and red the hottest. The great amount of detail revealed by the simulation even includes spattering (red dots).

problems and complex geometries where several packages are working in tandem, the code can maintain accuracy and efficiency.

The “arbitrary” in the code’s name refers to the ability to choose either the Lagrangian or Eulerian method of depicting an object on a mesh. The Lagrangian technique is used typically for structural simulations, while the Eulerian component is often used to simulate fluid flows. A Lagrangian mesh moves with the object, which greatly simplifies the related equations. These representations are accurate so long as the mesh remains intact, but in extreme cases—such as a material undergoing large deformations—the mesh can distort, tangle, or collapse, bringing the simulation to a stop. Eulerian mesh boundaries are distinct and fixed, and the object flows through the mesh.

ALE3D embodies ALE technology that Livermore has pioneered and where the Laboratory continues to advance the state of the art. The codes allow a user to not only switch between the Lagrangian and Eulerian techniques but even combine the two so that the mesh “relaxes” at the leading edge of the object. The amount of relaxation is determined by the user, who can “weight” the simulation so that more zones are forced into a specific area of interest, for greater accuracy at that spot. Supporting mesh relaxation broadens the scope of applications in comparison to codes that are restricted to Lagrangian- or Eulerian-only approaches.

For some applications, ALE3D can deliver accuracy similar to that of other simulation techniques but with as few as one-tenth the number of mesh elements, greatly reducing the amount of computer memory required. ALE3D operates on a wide variety of platforms, from laptops—for simple problems or debugging—to supercomputers. However, the ability to operate on massively parallel machines has always been a core requirement for the code, and industry and university collaborations using ALE3D-4I will be able to take advantage of Livermore’s HPC facilities to tackle complex problems quickly and efficiently.

### New Features for Additive Manufacturing

While work proceeds on ALE3D-4I, Noble’s team continues to enhance the full version of ALE3D. For example, engineers are implementing new features that will benefit laser-based additive manufacturing, where a laser melts a metal powder to build up the desired shape. Experiments at Livermore have shown that ALE3D does an excellent job of predicting how the metal powder melts. The simulations take into account factors such as the recoil force of vaporizing metal, changing surface tension, spattering, and cooling by evaporation and radiation. The code even captures the indentations made in the substrate, the flow of melted powder, and peak surface features. Many additional enhancements to ALE3D can be expected to grow from expanded application of the code with research partners in industry and academia.

In addition to adding new physics capabilities, the team is also making modifications to enable ALE3D to run well on Sierra and other next-generation supercomputers. Sierra, scheduled to arrive at Livermore later in 2017, will be at least five times more powerful than current Livermore supercomputers. (See *S&TR*, March 2017, pp. 4–11.) Noble says, “We’re confident that ALE3D-4I is going to fill a need that the engineering software industry can’t currently provide.” Filling that gap will undoubtedly help make U.S. industry more competitive in an increasingly challenging global marketplace.

—Arnie Heller

**Key Words:** additive manufacturing, ALE3D, ALE3D-4I, high-performance computing (HPC), High Performance Computing Innovation Center (HPCIC), Industrial Partnerships Office, innovation development funds, laser-based additive manufacturing, technology transfer.

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*In this section, we list recent patents issued to and awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory. For the full text of a patent, enter the seven-digit number in the search box at the U.S. Patent and Trademark Office's website (<http://www.uspto.gov>).*

### Patents

#### Detecting Pin Diversion from Pressurized Water Reactors Spent Fuel Assemblies

**Young S. Ham, Shivakumar Sitaraman**  
U.S. Patent 9,543,046 B2  
January 10, 2017

#### Graphene-Supported Metal Oxide Monolith

**Marcus A. Worsley, Theodore F. Baumann, Juergen Biener, Monika A. Biener, Yinmin Wang, Jianchao Ye, Elijah Tylski**  
U.S. Patent 9,543,569 B2  
January 10, 2017

#### Micro-Fluidic Partitioning Between Polymeric Sheets for Chemical Amplification and Processing

**Brian L. Anderson**  
U.S. Patent 9,550,186 B2  
January 24, 2017

#### Encapsulated Microenergetic Material

**Jeffery James Roberts, Roger D. Aines, Eric B. Duoss, Christopher M. Spadaccini, Kevin S. Vandersall**  
U.S. Patent 9,562,426 B2  
February 7, 2017

### Awards

Lawrence Livermore research engineer **Andy Pascall** received the **Best Presentation Award** for his talk at **World Materials Research Institutes Forum's (WMRIF's) 5th International Workshop for Young Scientists**. Pascall's presentation discussed his research into a new way to three-dimensionally print metal components by extruding a semisolid alloy from a printer nozzle, as toothpaste is squeezed from a tube.

WMRIF is an international organization with 50 member institutes, including several national laboratories. Pascall was chosen for the award by a review committee that considered criteria such as technical quality, presentation quality, potential impact, and the potential for benefiting the presenter. The award allows Pascall to visit any two WMRIF member institutions for two weeks at a time to learn more about their research and seek collaborative opportunities.

**Chris Barty**, chief technology officer of Lawrence Livermore's National Ignition Facility and Photon Science Directorate, has been named a 2017 **fellow** of the **Institute of Electrical and Electronics Engineers (IEEE)** for his contributions to ultrahigh-intensity lasers and the advancement of x-ray and gamma-ray science. Fellow is the highest grade of IEEE membership and is awarded to a person with an outstanding record of accomplishments in any of the IEEE fields of interest.

Barty also currently serves as chair of the International Committee on Ultra-High Intensity Lasers. He has published more than 200 manuscripts and presented more than 200 invited talks over the years. His work has spanned lasers, optics, materials science, medicine, chemistry, engineering, and physics. At Livermore, he has served as the chief scientist for the Laser Science and Technology Program and was architect and first director of the mission-focused Photon Science and Applications Program.

**Jay Zucca**, Lawrence Livermore geophysicist and principal deputy of the Global Security Principal Directorate, was presented

with the **National Nuclear Security Administration's (NNSA's) Gold Medal of Excellence for Distinguished Service**, which is the highest honorary award granted by NNSA. Bestowed for his 29 years of demonstrating outstanding scientific contributions and leadership toward U.S. global and nuclear security and nuclear explosion monitoring, the award also recognizes his work on programs and treaties, such as the Laboratory's Ground-Based Nuclear Explosion Monitoring (GNEM) Program and the Preparatory Commission for the Comprehensive Nuclear-Test-Ban Treaty Organization (CTBTO).

Zucca led the GNEM Program's scientists and engineers in developing methods for monitoring underground nuclear explosions. He participated in the conference on disarmament that was part of CTBTO negotiations and, for nearly the past 20 years, has been a member of the U.S. delegation to the CTBTO's Working Group B, the international body that seeks to resolve technical issues related to the treaty.

**Fusion Power Associates (FPA)** has selected **Joe Kilkenny**—scientific diagnostic leader of Lawrence Livermore's National Ignition Facility (NIF) and vice president for high-energy-density physics at General Atomics—to receive a 2016 **Leadership Award**. FPA Leadership Awards have been presented since 1980 to individuals who have shown outstanding leadership qualities in accelerating the development of fusion.

After coming to the Laboratory in 1983, Kilkenny led the Inertial Confinement Fusion Program from 1995 to 2001, helping spawn the creation of NIF. He is also recognized for his leadership in developing instruments for NIF's National Diagnostics Program. For nearly four decades, Kilkenny has been a leader in the field of inertial confinement fusion, pioneering work at major laser facilities on hydrodynamic instabilities, opacity, thermal and suprathermal electron transport, and advanced diagnostics.



### Ready, Set, Innovate! Entrepreneurship Flourishes at the Laboratory

For 65 years, Lawrence Livermore has embraced its role as a venue for scientific research and development, a proving ground for new technology, and an advocate for transferring technology to the private sector. Livermore actively cultivates a culture of entrepreneurship to ensure that appropriate innovations find a purpose beyond Laboratory gates. This commercialization enhances U.S. economic security at a local, state, and national level. The Laboratory's Industrial Partnerships Office (IPO) assists scientists and engineers with the myriad aspects of technology transfer, such as licensing agreements, nondisclosure contracts, invention disclosures, patent applications, business plans, intellectual property protection, funding applications, and go-to-market strategies. Annually, Livermore-developed technologies generate \$300 million in product sales, earning the Laboratory \$8 million in licensing fees and royalties. With more than 1,000 active agreements and just as many patents and patent applications, IPO also oversees more than 140 active commercial licenses and cooperative research and development agreements. To recognize scientists whose inventiveness has made significant contributions to the Laboratory and the private sector, IPO established the Entrepreneurs' Hall of Fame in 2012. In a broad range of commercial fields—from pioneering laser peening and satellite imaging technology to new computer simulations and cybersecurity solutions—Hall of Fame inductees continue to make an impact in U.S. industries while maintaining their Laboratory ties in ways that enhance Livermore's culture of entrepreneurship.

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- *Materials and computation researchers join forces to accelerate the process of materials discovery, optimization, and scaleup through machine learning and big-data analytics.*
- *Scientists provide new nanoscale insight into high-explosive detonation processes.*

Science & Technology Review  
Lawrence Livermore National Laboratory  
P.O. Box 808, L-664  
Livermore, California 94551

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